Yoong-Kee Choe

List of Publications by Year
in descending order

60 papers	2,356 citations	218592 26 h-index	206029 48 g-index
61 all docs	61 docs citations	61 times ranked	2671 citing authors

#	Article	IF	Citations
1	Synthesis, structure and properties of trivalent and pentavalent tricarbabismatranes. Chemical Communications, 2022, 58, 6614-6617.	2.2	3
2	Mechanistic investigation on ethanolâ€toâ€butadiene conversion reaction over metal oxide clusters. International Journal of Quantum Chemistry, 2021, 121, e26494.	1.0	13
3	Theoretical study of the side reactions of the catalytic conversion of ethanol to butadiene on metal oxide catalysts. Catalysis Communications, 2021, 149, 106239.	1.6	2
4	First-principles molecular dynamics simulation study on Ti4+ ion in aqueous sulfuric acid. AIP Advances, 2021, 11, 035224.	0.6	2
5	Theoretical Study of the Mechanism for the Reaction of Trimethylaluminum with Ozone. ACS Omega, 2021, 6, 26282-26292.	1.6	5
6	[Pd(4-RSi-IPr)(allyl)Cl]/KCO/EtOH: A highly effective catalytic system for the Suzuki-Miyaura cross-coupling reaction. Journal of Organometallic Chemistry, 2021, 954-955, 122096.	0.8	5
7	Nâ€Aryl and Nâ€Alkyl Carbamates from 1 Atmosphere of CO₂. Chemistry - A European Journal, 2021, 27, 18066-18073.	1.7	12
8	Suppressing vanadium crossover using sulfonated aromatic ion exchange membranes for high performance flow batteries. Materials Advances, 2020, 1, 2206-2218.	2.6	22
9	Fundamental roles of ZnO and ZrO₂in the conversion of ethanol to 1,3-butadiene over ZnOâ€“ZrO₂/SiO₂. Catalysis Science and Technology, 2020, 10, 7531-7541.	2.1	13
10	Structure dependency of the reactivity of aromatic hydrocarbons involving the formation of oxygenated polycyclic aromatic hydrocarbons (OPAHs). Chemical Physics Letters, 2020, 754, 137652.	1.2	4
11	Turning Harmful Deposition of Metal Impurities into Activation of Nitrogen-Doped Carbon Catalyst toward Durable Electrochemical CO₂ Reduction. ACS Energy Letters, 2019, 4, 2343-2350.	8.8	23
12	The energetics of phosphoric acid interactions reveals a new acid loss mechanism. Journal of Materials Chemistry A, 2019, 7, 9867-9876.	5.2	83
13	Mechanistic Details on the Conversion of Siâ€“O to Siâ€“C Bonds Using Metal Hydrides: A Density Functional Theory Study. European Journal of Inorganic Chemistry, 2019, 2019, 1335-1342.	1.0	1
14	[Pd(4-R₃Si-IPr)(allyl)Cl], a Family of Silyl-Substituted Pdâ€“NHC Complexes: Catalytic Systems for the Buchwaldâ€“Hartwig Amination. Organometallics, 2019, 38, 375-384.	1.1	22
15	DFT Studies of Perfluorosulfonic Acid Ionomer Degradation in Fuel Cells. Journal of Physical Chemistry C, 2018, 122, 20135-20143.	1.5	15
16	Alkoxysilane production from silica and dimethylcarbonate catalyzed by alkali bases: A quantum chemical investigation of the reaction mechanism. Inorganica Chimica Acta, 2018, 482, 70-76.	1.2	13
17	Tris(pentafluorophenyl)boraneâ€Catalyzed Reactions of Siloxanes: A Combined Experimental and Computational Study. European Journal of Organic Chemistry, 2017, 2017, 4922-4927.	1.2	9
18	First-principles molecular dynamics simulation study on electrolytes for use in redox flow battery. AIP Conference Proceedings, 2017, , .	0.3	0

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19	Effect of Organic Cations on Hydrogen Oxidation Reaction of Carbon Supported Platinum. Journal of the Electrochemical Society, 2016, 163, F1503-F1509.	1.3	29
20	Computational modeling study on polymer electrolyte membranes for fuel cell applications. AIP Conference Proceedings, 2016, , .	0.3	0
21	Olefin hydrosilylation catalyzed by cationic nickel(<scp>ii</scp>) allyl complexes: a non-innocent allyl ligand-assisted mechanism. Chemical Communications, 2016, 52, 6723-6726.	2.2	32
22	Systematic Alkaline Stability Study of Polymer Backbones for Anion Exchange Membrane Applications. Macromolecules, 2016, 49, 3361-3372.	2.2	287
23	An operationally flexible fuel cell based on quaternary ammonium-biphosphate ion pairs. Nature Energy, 2016, 1, .	19.8	206
24	First-Principles Molecular Dynamics Study of a Hydrocarbon Copolymer for Use in Polymer Electrolyte Membrane Fuel Cells. Journal of Physical Chemistry C, 2016, 120, 13398-13405.	1.5	6
25	Chemical degradation mechanisms of membranes for alkaline membrane fuel cells. AIP Conference Proceedings, 2015, , .	0.3	0
26	A DFT Study on the Dissociation Property of Sulfonic Acids with Different Neighboring Pendants in Polymer Electrolyte Membranes. , 2015, , .		0
27	An adaptive finite-element method for large-scale ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2015, 17, 31444-31452.	1.3	18
28	Theoretical studies on the degradation of hydrocarbon copolymer ionomers used in fuel cells. Journal of Membrane Science, 2015, 487, 229-239.	4.1	32
29	Theoretical Studies of Pendant Effects on the Properties of Sulfonated Hydrocarbon Polymer Electrolyte Membranes. Journal of Physical Chemistry C, 2015, 119, 11362-11369.	1.5	7
30	Alkaline Stability of Benzyl Trimethyl Ammonium Functionalized Polyaromatics: A Computational and Experimental Study. Chemistry of Materials, 2014, 26, 5675-5682.	3.2	152
31	Ab initio studies on the proton dissociation and infrared spectra of sulfonated poly(ether ether) Tj ETQq1 1 0.784314 rgBT /Overlock	1.3	20
32	Resonance Stabilized Perfluorinated Ionomers for Alkaline Membrane Fuel Cells. Macromolecules, 2013, 46, 7826-7833.	2.2	90
33	Molecular Design Aspect of Anion Exchange Polymer Electrolytes. ECS Transactions, 2013, 58, 417-423.	0.3	0
34	Iterative diagonalization of symmetric matrices in mixed precision and its application to electronic structure calculations. Computer Physics Communications, 2012, 183, 980-985.	3.0	11
35	Synthesis, Structure, and Reactivity of Hydridoiridium Complexes Bearing a Pincerâ€Type PSiP Ligand. Chemistry - an Asian Journal, 2011, 6, 2512-2521.	1.7	80
36	Understanding properties of copoly(arylene ether nitrile)s high-performance polymer electrolyte membranes for fuel cells from molecular dynamics simulations. Theoretical Chemistry Accounts, 2011, 130, 555-561.	0.5	3

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37	An Ab Initio Modeling Study on a Modeled Hydrated Polymer Electrolyte Membrane, Sulfonated Polyethersulfone (SPES). Journal of Physical Chemistry B, 2010, 114, 2411-2421.	1.2	38
38	Proton Dynamics in a Polymer Electrolyte Membrane, Sulfonated Polyether Sulfone (SPES): A Computational Study. ECS Transactions, 2009, 25, 1075-1083.	0.3	2
39	Vibrational analysis of aqueous sulfuric acid: A computational study. International Journal of Quantum Chemistry, 2009, 109, 1984-1990.	1.0	8
40	A unique Biâ€“Bi bond forming reaction using organobismuth oxides and phosphorus compounds bearing a P(î€O)H group. Chemical Communications, 2009, , 6168.	2.2	32
41	Nature of proton dynamics in a polymer electrolyte membrane, nafion: a first-principles molecular dynamics study. Physical Chemistry Chemical Physics, 2009, 11, 3892.	1.3	93
42	Nature of Water Transport and Electro-Osmosis in Nafion: Insights from First-Principles Molecular Dynamics Simulations under an Electric Field. Journal of Physical Chemistry B, 2008, 112, 11586-11594.	1.2	51
43	Multinuclear palladium compounds containing palladium centers ligated by five silicon atoms. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 7758-7763.	3.3	47
44	First-principles molecular dynamics study on aqueous sulfuric acid solutions. Journal of Chemical Physics, 2007, 126, 154510.	1.2	55
45	Theoretical study of the electronic spectra of oxidized and reduced states of lumiflavin and its derivative. Journal of Computational Chemistry, 2007, 28, 727-739.	1.5	36
46	Electrical property of a sulfuric acidâ€“water mixture from the first-principles molecular dynamics simulation. Computer Physics Communications, 2007, 177, 38-39.	3.0	3
47	Effect of the axial cysteine ligand on the electronic structure and reactivity of high-valent iron(IV) oxo-porphyrins (Compound I): A theoretical study. Journal of Computational Chemistry, 2005, 26, 1600-1611.	1.5	15
48	Isolation of aSe-Nitrososelenol:Â A New Class of Reactive Nitrogen Species Relevant to ProteinSe-Nitrosation. Journal of the American Chemical Society, 2004, 126, 13238-13239.	6.6	46
49	Calculation of packing structure of methanol solid using ab initio lattice energy at the MP2 level. Chemical Physics Letters, 2003, 369, 597-604.	1.2	15
50	Effect of Substituents on the Thermal Decomposition of Diazirines:Â Experimental and Computational Studies. Journal of Organic Chemistry, 2003, 68, 7471-7478.	1.7	32
51	Theoretical identification ofC20carbon clusters:â€ƒPrevalence of the monocyclic isomer and existence of the smallest fullerene and bowl isomer. Physical Review B, 2003, 67, .	1.1	22
52	A comparison of the photochemical reactivity of N@C60 and C60: photolysis with disiliraneElectronic supplementary information (ESI) available: experimental results. See http://www.rsc.org/suppdata/cc/b3/b309470g/. Chemical Communications, 2003, , 2940.	2.2	30
53	A CASCI-MRMP method based on Kohnâ€”Sham orbitals. Molecular Physics, 2002, 100, 729-745.	0.8	27
54	Intruder state avoidance multireference MÃ¸ller-Plesset perturbation theory. Journal of Computational Chemistry, 2002, 23, 957-965.	1.5	186

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55	Multireference MÃ¸llerâ€“Plesset method with a complete active space configuration interaction reference function. Journal of Chemical Physics, 2001, 115, 621-629.	1.2	59
56	Identifying and removing intruder states in multireference Mo/llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2001, 114, 3913-3918.	1.2	61
57	On the performance of diagrammatic complete active space perturbation theory. Journal of Chemical Physics, 2000, 113, 7773-7778.	1.2	6
58	Theoretical study of the electronic ground state of iron(II) porphine. II. Journal of Chemical Physics, 1999, 111, 3837-3845.	1.2	76
59	Theoretical Study of the Q and B Bands of Free-Base, Magnesium, and Zinc Porphyrins, and Their Derivatives. Journal of Physical Chemistry A, 1999, 103, 1894-1904.	1.1	157
60	Theoretical study of the electronic ground state of iron(II) porphine. Chemical Physics Letters, 1998, 295, 380-388.	1.2	39